

then investigate the elastic properties of membranes, especially the Gaussian curvature modulus.

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Molecular Level Modeling of the Effects of Charge and Sugars on the Phase Equilibrium of Model Lipid Bilayers

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We present a mean-field theoretical molecular model capable of addressing the disparity in results drawn from experiments studying the structural and thermodynamic characteristics within multicomponent anionic model membranes. The experiments were drawn under identical system conditions, differing only in lipid preparation method—electrophoresis, in the presence of sugar solutions, versus a gentle hydration protocol, absent of sugars. The discrepancies in the membrane phase behavior were noted, but left uncharacterized due to constraints on the experimental conditions that limited the yields necessary to evaluate a comparison drawn between the techniques.

Such experimental limitations highlight the utility of our theory, from which we can capture the non-trivial coupling between organizational and physicochemical properties within the system. We use a molecular model to quantify the isolated and net contributions of glucose, sucrose, and counterion distribution to the stability of phase-coexistence regions in ternary anionic membranes comprised of dipalmitoylphosphatidylcholine (DPPC), anionic dioleoylphosphatidylglycerol (DOPG), and cholesterol. The theory is based on a free energy formulation that explicitly accounts for the architecture and charge distribution of all system molecules, while treating the intermolecular interactions within a mean-field approach. A distinguishing attribute of our theory is the rigorous construction of all system components from a molecular foundation, realistically characterizing the system's physics on the scale of the monomer. The size and shape of each monomeric unit are treated explicitly, and all possible conformations, as well as a comprehensive set of translational and rotational states, are included.

As delineated in this work, anionic lipid head-regions present hydroxyl groups capable of forming hydrogen-bond networks. The introduction of sugar molecules motivates strong interactions with these networks, tremendously disrupting the stability of phase coexistence regions. Screening of counterions partially alleviates this effect.

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Edge Structure of through Pore in Lipid Membrane

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Theoretical model of edge structure of through pore in lipid membrane was developed. We assumed that membrane monolayers are not necessary in close contact with each other everywhere; instead, hydrophobic void can appear between monolayers of the membrane near the pore edge. If formed, the void is supposed to be filled by organic solvent or low-polarity impurities, which are usually present in artificial and cell membranes. The monolayer of pore edge was divided to three regions: almost vertical monolayer, almost horizontal monolayer, and horizontal monolayer of bilayer part of the membrane. All three regions were assumed continuously conjugated. Pore line tension was calculated in the framework of theory of elasticity of liquid crystals adapted to lipid membranes, by taking into account splay and tilt deformations. Line tension depends on the value of surface tension at the boundary of lipid tails with the void. For sufficiently high surface tension the void collapses. Calculated values of pore edge line tension are in good agreement with available experimental data both for membranes containing and lacking organic solvent or low-polarity impurities.

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Bolalipid Membranes: Elasticity Theory Approach

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Bolalipids is a new and very intriguing and promising object for the investigations. Bolalipids are the main component of extremophilic bacteria's cell mem-

brane and mostly responsible their exceptional stability and vitality under the high temperature, pressure and environment acidity. As opposed to "conventional" lipids bolalipids are composed of two polar head connected by two hydrocarbonic tails and can either pierce through the whole membrane or form a U-shape configurations. Bolalipids' investigation is at its opening stage. There is lack of experimental data on the model membranes, on the theoretical side the researches are limited by computer simulations data and some microscopical models. However, for the effective progress in the investigation of the bolalipid membranes the elasticity theory should be developed. Similar theory applied to the conventional lipid membranes gives results that are in an excellent agreement with the experimental data. That is why we have chosen the way of construction the effective elasticity theory of bolalipids on the basis of conventional lipid one.

In the present work we constructed the phenomenological elasticity theory of the bolalipid membranes. The set of all feasible types of deformations are found. It have been shown that, unlike to conventional lipids, bolalipid's elasticity theory demands two bending moduli. Possible experiments for the determining of the elastic moduli are suggested. Theory takes into account the presence of the two configurations of bolalipids in the membrane: U-shape and O-shape configurations. The way of the experimental determination of the ratio of these configurations is proposed.

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Physical Properties and Membrane Packing in Hybrid Archaeosomes

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In this study, we have characterized the physical properties of liposomes made of archaeal bipolar tetraether lipids (BTL) and "conventional" monopolar diester lipids (termed as hybrid archaeosomes). We used the polar lipid fraction E (PLFE) isolated from the thermoacidophilic archaeon *Sulfolobus acidocaldarius* as the BTL component of the hybrid archaeosomes. Hybrid archaeosomes were made by extrusion with the particle size ranging from 100–300 nm. Dynamic light scattering and zeta potential measurements showed that the presence of PLFE greatly stabilizes liposomes. The steady-state polarization of DPH fluorescence in PLFE/PC mixtures decreases with increasing temperature (18–56°C) in a molar ratio dependent manner. At low temperatures, hybrid archaeosomes have membrane packing, as inferred from DPH polarization, similar to that in gel state of disaturated PC bilayers. At the high temperature end, membrane packing of the hybrid archaeosomes is significantly tighter than that of PC fluid state. A similar conclusion can be drawn from the studies using Laurdan's generalized polarization. Additionally, due to tight membrane packing, drug release from hybrid archaeosome is much slower than from liposomes composed of only diester lipids. Confocal fluorescence microscopy showed that these hybrid archaeosomes can be taken up by live cells (e.g., MCF-7 breast cancer cells) and deliver entrapped drug molecules to the cell's nucleus, but with a rate significantly lower than that obtained from conventional diester liposomes.

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Temperature-Dependent Lipid Phase Transitions Occurring in Higher Organisms

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Previously published data concerning the temperature dependence of the neural responses of frog, squid and rat have been examined for unusual features occurring at the gestation temperature, T_g , of such organisms. The temperature dependencies of the resting potential and action potential of frog and squid exhibit behaviors that strongly suggest the onset of a membrane state change when $T > T_g$. Anomalies in the flow of current in the rat ganglion lead to a similar conclusion. Membranes formed of whole lipid extracts from various organisms, including extracts from neural tissues, have been observed to exhibit a phase transition at a temperature $T^* = T_g$. Based on approximations to the classic Hodgkin-Huxley equations, analysis of axonal response indicates that observed changes in the resting potential and peak of the action potential reflect chemo-mechanical coupling between voltage-switchable ion channels and temperature-linked, lipid phases of the plasma membrane. The behavior of the resting potential and action potential when $T > T_g$ can be rationalized by postulating the emergence of a different lipid state that alters channel properties. The change in neural properties with increasing temperature for these animals has an activation energy of approximately 26 kcal/mole. Short exposure to temperatures above T_g alters the stability of the channels, whereas elevating the temperature for longer periods appears to result in irreversible degradation of the tissue.